Orbital Correlations, Frustration, and Self-Organization

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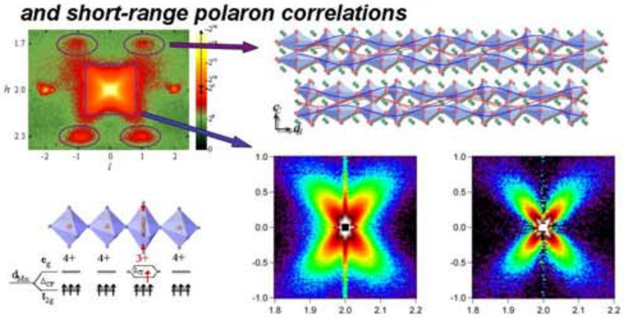
Motivation

- ***Need to understand the role of orbital occupation on the underlying physical properties, e.g., superconductivity, colossal magnetoresistance (CMR), ferroelectricity, spin ladder formation etc.***
- ***Combine variety of techniques to probe orbital configuration***
  - ***Elastic diffuse scattering: nanoscale self-organization e.g. stripes, dimerization, phase separation***
  - ***Elastic neutron and X-ray diffraction: average structure***
  - ***Inelastic neutron scattering: energy scale of the interactions***

Layered CMR manganites

- ***Diffuse scattering reveals Jahn-Teller polarons and short-range polaron correlations***



- ***Comprehensive temperature dependent studies enable a direct measure of the polaron population***

Future Directions

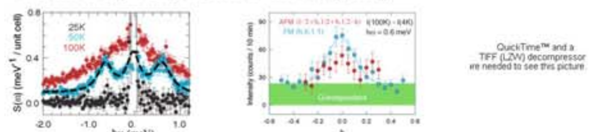
➢ *Determine origin of competing order parameters*

➢ *Determine fluctuations associated with reentrant charge order*

S.N. Ancona et al., to be published 2006

$La_{1-x}Sr_xCoO_3$

- ***Similar behavior as manganites, e.g. concomitant insulator-metal and ferromagnetic transition***
- ***Spin-state of Co^{3+}, electron-lattice coupling, tunable by temperature and doping.***



- ***Inelastic and elastic neutron scattering:***
  - ***Emergence of low-energy excitation due to temperature induced spin-state transition***
  - ***Ferro- and antiferromagnetic correlations due to dynamic, short-range orbital ordering***

Future Directions

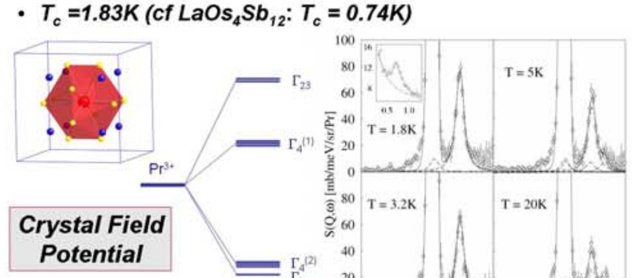
➢ *Evolution of ferromagnetic/charge/orbital order with doping*

➢ *Measure diffuse scattering due to Co^{3+} Jahn-Teller polarons*

D. Phelan et al., Phys. Rev. Lett. 96, 027201 (2006)

Skutterudites

- ***$PrOs_4Sb_{12}$ is a heavy fermion superconductor.***
- ***T_c =1.83K (cf $LaOs_4Sb_{12}$: T_c = 0.74K)***



$$H_{CF} = B_4\left(O_4^0 + 5O_4^4\right) + B_6\left(O_6^0 - 21O_6^4\right) + \boxed{B_6^t\left(O_6^2 - O_6^6\right)}$$

- ***From inelastic neutron scattering:***
  - ***The Pr^{3+} ground state is a Γ_1 singlet.***
  - ***T_c is enhanced by inelastic quadrupolar scattering***

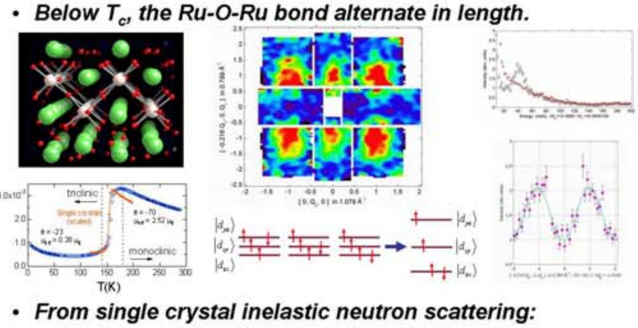
Future Directions

➢ *Explore s-f interaction through crystal field relaxation*

E.A. Goremychkin et al., Phys. Rev. Lett. 93, 157003 (2004)

Ruthenates

- ***$La_4Ru_2O_{10}$ has a first-order phase transition at 160K.***
- ***Corner-shared RuO_6 octahedra form a corrugated plane.***
- ***Below T_c, the Ru-O-Ru bond alternate in length.***



- ***From single crystal inelastic neutron scattering:***
  - ***A spin gap of 40meV develops below the transition.***
  - ***Modulations in Q indicate the formation of S=1 dimers***
  - ***The results can be explained by t_{2g} orbital ordering.***

Future Directions

➢ *Investigate other candidates of Orbital Peierls distortions*

P. Khalifah et. al., Science 297, 2237 (2002)

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